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On quadrature error expansions. Part I*

J.N. LYNESS
Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439, U.S.A.

Elise DE DONCKER-KAPENGA
Computer Science Department, Western Michigan University, Kalamazoo, MI 49008, U.S.A.

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Abstract: We treat the theory of numerical quadrature over a square using an m^2 copy $Q^{(m)}f$ of a one-point quadrature rule. For some integrand functions the quadrature error $Q^{(m)}f - If$ may be expressed as an asymptotic expansion in inverse powers of m or other simple functions of m. We determine in some cases the nature of this expansion and derive integral representations for both the coefficients and the remainder term. In this part we deal only with smooth functions and those having algebraic line singularities along edges. In some of these cases the form is already known but some of the integral representations are new. These results form the basis for Part II in which new expansions, for integrands having algebraic singularities along intersecting edges and point algebraic singularities at the vertices will be presented.

1. Introduction

One familiar method of one-dimensional numerical quadrature is Romberg Integration. This is based on the classical Euler–Maclaurin asymptotic expansion which is valid when the integrand function and its early derivatives are integrable over the integration interval. This asymptotic expansion is easy to prove and is well known.

It is only recently that investigators have turned to the problem of generalizing the procedure to integrand functions having singularities. Since then several results have been established relating to integration over (N-dimensional) hypercubes and simplices. The significant difficulty has usually been the construction of the corresponding analog of the Euler–Maclaurin asymptotic expansion. These efforts have been characterized by long and complicated formulas [1]. In fact at first glance, it seems that progress is made only as and when simple notation is constructed.

In Section 2 we treat only one-dimensional integration over a finite interval taken to be [0, 1] using the off-set m-panel trapezoidal rule defined by

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$$Q_\alpha^{(m)} f = \frac{1}{m} \sum_{j=0}^{m-1} f\left(\frac{j+\alpha}{m}\right), \quad 0 \leq \alpha \leq 1 . \tag{1.1}$$

This is the m-copy of the one-point rule $Q_\alpha f = f(\alpha)$. In Section 3 we treat integration over the square

$$H_2\colon\ 0 \leq x \leq 1 ; \quad 0 \leq y \leq 1 . \tag{1.2}$$

Here we use the m^2-copy of the rule $Q_{\alpha,\beta} f = f(\alpha, \beta)$ namely

$$Q_{\alpha,\beta}^{(m)} f = \frac{1}{m^2} \sum_{j=0}^{m-1} \sum_{k=0}^{m-1} f\left(\frac{j+\alpha}{m}, \frac{k+\beta}{m}\right), \quad \alpha, \beta \in H_2 . \tag{1.3}$$

The familiar m-panel trapezoidal rule can be expressed in the form

$$Qf = \tfrac{1}{2}(Q_0^{(m)} f + Q_1^{(m)} f) . \tag{1.4}$$

In general, the m-copy of any one-dimensional quadrature rule

$$Gf = \sum_{l=1}^{\nu} w_l f(\beta_l) \tag{1.5}$$

can be expressed as

$$G^{(m)} f = \sum_{l=1}^{\nu} \frac{w_l}{m} \sum_{j=0}^{m-1} f\left(\frac{j+\beta_l}{m}\right) = \sum_{l=1}^{\nu} w_l Q_{\beta_l}^{(m)} f . \tag{1.6}$$

It follows that an Euler–Maclaurin expansion for any rule may be constructed from the corresponding expansions for individual one-point rules by simply taking a weighted sum. It is sufficient then, in developing the theory, to treat only one-point rules.

When $G(x)$ and its first p derivatives are integrable a trivial extension of the classical Euler–Maclaurin expansion is

$$Q_\beta^{(m)} G - IG = \sum_{s=1}^{p-1} \frac{B_s}{m^s} + R_p(m) , \tag{1.7}$$

where B_s is independent of m and $R_p(m) = O(m^{-p})$. Integral representations for B_s and $R_p(m)$ are well known and are given below. In this paper we treat this formula and generalizations of this formula for integrand functions of the following characters.

Theorem 2.1	$G(x)$,
Theorem 2.4	$f_\lambda(x) = x^\lambda$,
Theorem 2.5	$F_{\lambda,0}(x) = x^\lambda G(x)$,
Theorem 2.6	$f_{0,\mu}(x) = (1-x)^\mu$,
Theorem 2.8	$F_{\lambda,\mu}(x) = x^\lambda (1-x)^\mu G(x)$,
Theorem 3.2	$F_\lambda(x, y) = x^\lambda G(y)$,
Theorem 3.4	$G(x, y)$,
Theorem 3.5	$\Gamma_\lambda(x, y) = x^\lambda G(x, y)$.

Here $G(x)$ and $G(x, y)$ are functions whose early derivatives are continuous and λ and μ are not integers.

The fundamental theorems are the first two and Theorem 3.5. The other theorems are derived from these by the appropriate use of subtraction functions, reflection, and formula (3.4) which can be used to form the two-dimensional product of two independent one-dimensional expansions.

We provide an integral representation for all the terms in the expansion. Since these are quite complicated we have had to introduce concise notation (3.19)–(3.21). While the nature of most of the expansions is already known, most of the integral representations for the coefficients and the remainder terms are new. These representations will be needed to construct new expansions in Part II.

In this paper and its sequel, we have adhered to several notational conventions.

(a) The constants in the expansions are denoted by the letter A, B, C, or E with a subscript and a set of arguments. The subscript denotes the inverse power of m in the cofactor. The arguments denote respectively the regions ($[0, 1]$ or H_2), the rule (Q_α, Q_β or $Q_{\alpha,\beta}$) and the integrand function (G, F_λ, etc.) in whose asymptotic expansion this is a term. In Section 3, $Q_{\alpha,\beta}$ is suppressed.

(b) Elements of remainder terms are denoted by $R_p(m; \ldots)$; the subscript p denotes that this is $\mathrm{O}(m^{-p})$ or of lower order. Arguments other than m have the same meaning as in (a) above.

We have also adhered to certain self imposed constraints. These include:

(i) We do not consider at all the expansions for integrands having arbitrarily located point (or line) singularities. For some such integrands, expansions involving the ζ function (Hurwitz) exist, but are presently considered to be too complicated for practical use.

(ii) We do not consider expansions for functions having logarithmic singularities. Some of these may be obtained from those given here by differentiation with respect to incidental parameters such as λ.

(iii) We have not considered special cases in which some coefficients vanish because of special properties of the quadrature rule, symmetry or other properties of the integrand function and so on.

2. One-dimensional expansions

Let $G(x)$ be an integrand function and

$$Q_\beta G = G(\beta)\,, \quad 0 \leq \beta \leq 1\,, \tag{2.1}$$

be a one-point quadrature rule approximation to the integral

$$IG = \int_0^1 G(x)\,\mathrm{d}x\,. \tag{2.2}$$

The m-copy of Q_β is defined by

$$Q_\beta^{(m)} G = \frac{1}{m} \sum_{k=0}^{m-1} G((\beta + k)/m)\,. \tag{2.3}$$

Theorem 2.1. *When $G(x)$ and its first p derivatives are an integrable in* $[0, 1]$ *and* $p \geqslant 1$,

$$Q_\beta^{(m)}G - IG = \sum_{s=1}^{p-1} \frac{B_s([0,1], Q_\beta, G)}{m^s} + R_p(m; [0,1], Q_\beta, G) \tag{2.4}$$

where B_s is independent of m and $R_p = \mathrm{O}(m^{-p})$.

This is a well known minor generalization of the classical Euler–Maclaurin summation formula. The integral representations of the coefficients depend on the rule Q_β through one of two kernel functions.

Definition 2.2.

$$h_s^{[1]}(\beta, t) = c_s(\beta) = B_s(\beta)/s!\,, \qquad s \geqslant 0\,, \tag{2.5}$$

$$h_s^{[0]}(\beta, t) = h_s(\beta, t) = (B_s(\beta) - \bar{B}_s(\beta - t))/s!\,, \quad s \geqslant 1\,, \tag{2.6}$$

where $B_s(x)$ is the Bernoulli polynomial of degree s and $\bar{B}_s(x)$ is the associated Bernoulli function which coincides with $B_s(x)$ in the interval $(0, 1)$ and has unit period.

Two properties of these coefficients are

$$h_p(\beta, t) = h_p(\beta, t+1) \quad \text{for all } t,\ p = 1, 2, 3, \ldots . \tag{2.7}$$

$$c_p(\beta) = \int_0^1 h_p(\beta, t)\,\mathrm{d}t\,, \quad p = 1, 2, 3, \ldots . \tag{2.8}$$

In terms of these quantities, the coefficients in (2.4) are

$$B_s([0,1], Q_\beta, G) = c_s(\beta) \int_0^1 G^{(s)}(t)\,\mathrm{d}t\,, \qquad s = 0, 1, \ldots, \tag{2.9}$$

$$R_p(m; [0,1], Q_\beta, G) = m^{-p} \int_0^1 h_p(\beta, mt) G^{(p)}(t)\,\mathrm{d}t\,, \quad p = 1, 2, \ldots . \tag{2.10}$$

It is convenient to define

$$R_0(m; [0,1], Q_\beta, G) = Q_\beta^{(m)}G \tag{2.11}$$

and to treat $h_0(\beta, mt)$ as a delta function. Note that

$$\begin{aligned} &B_0([0,1], Q_\beta, G) = IG\,, \\ &B_s([0,1], Q_\beta, G) = c_s(\beta)(G^{(s-1)}(1) - G^{(s-1)}(0))\,, \quad s = 1, 2, \ldots . \end{aligned} \tag{2.12}$$

Theorem 2.1 is valid when $G(x)$ and its first p derivatives are integrable. Thus it can be applied to the function defined by

$$f_\lambda(x) = x^\lambda\,, \quad \lambda > -1 \tag{2.13}$$

only so long as $p \leqslant \lambda$. A variant of expansion (2.4) is required for higher values of p. This is given in (2.17) below. The nature of the series is well known. (See for example [2,5]). We shall require an integral representation for the remainder term. Since the derivation of this simple result employs techniques used later in a more complicated context, we outline the proof.

Lemma 2.3.

$$\int_1^m f_\lambda^{(s)}(x)\,dx = \begin{cases} (m^{\lambda+1-s}-1)\displaystyle\int_0^1 f_\lambda^{(s)}(x)\,dx\,, & s<\lambda+1\,,\\ (m^{\lambda+1-s}-1)\displaystyle\int_\infty^1 f_\lambda^{(s)}(x)\,dx\,, & s>\lambda+1\,,\\ -\log_2 m\displaystyle\int_2^1 f_\lambda^{(s)}(x)\,dx\,, & s=\lambda+1\,,\end{cases} \tag{2.14}$$

and

$$\frac{1}{m^{\lambda+1}}\int_1^m h_s(\alpha,t)f_\lambda^{(s)}(t)\,dt$$
$$= \frac{1}{m^{\lambda+1}}\int_1^\infty h_s(\alpha,t)f_\lambda^{(s)}(t)\,dt + \frac{1}{m^s}\int_\infty^1 h_s(\alpha,mt)f_\lambda^{(s)}(t)\,dt\,,\quad s>\lambda+1\,. \tag{2.15}$$

These elementary formulas can be verified by setting $f_\lambda(x)=x^\lambda$.

In view of the different lower limits of integration occurring under different conditions in these formulas, we make another *notational definition*.

$$a_\nu = \begin{cases} 0, & \nu<0\,,\\ 2, & \nu=0\,,\\ \infty, & \nu>0\,.\end{cases} \tag{2.16}$$

The reader will note that on the right hand sides of (2.14) and (2.15) the lower limits 0, 2, ∞ may all be replaced by $a_{s-\lambda-1}$.

Theorem 2.4. *Let $f_\lambda(x)=x^\lambda$ where $\lambda>-1$. Let $Q_\alpha^{(m)}f_\lambda$ be finite. Then*

$$Q_\alpha^{(m)}f_\lambda = \frac{E_{\lambda+1}([0,1],Q_\alpha,f_\lambda)}{m^{\lambda+1}} + \sum_{s=0}^{p-1}\frac{B_s([0,1],Q_\alpha,f_\lambda)}{m^s}$$
$$+ R_p(m;[0,1],Q_\alpha,f_\lambda)\,,\quad \forall p\geq\lambda+1\,, \tag{2.17}$$

where $E_{\lambda+1}$ and B_s are independent of m and $R_p=O(m^{-p})$. The values of these coefficients are

$$B_s([0,1],Q_\alpha,f_\lambda) = c_s(\alpha)\int_{a_{s-\lambda-1}}^1 f_\lambda^{(s)}(t)\,dt\,,\quad s=0,1,\ldots, \tag{2.18}$$

$$R_s(m;[0,1],Q_\alpha,f_\lambda) = \frac{1}{m^s}\int_{a_{s-\lambda-1}}^1 h_s(\alpha,mt)f_\lambda^{(s)}(t)\,dt\,,\quad s=1,2,\ldots, \tag{2.19}$$

$$E_{\lambda+1}([0,1],Q_\alpha,f_\lambda) = R_{\bar s}(1;[0,1],Q_\alpha,f_\lambda)$$
$$-\sum_{s=\bar s}^{\bar p-1}B_s([0,1],Q_\alpha,f_\lambda) - R_{\bar p}(1;[0,1],Q_\alpha,f_\lambda)\,, \tag{2.20}$$

for any values of $\bar{s}$ *and* $\bar{p}$ *satisfying* $0 \leq \bar{s} < \lambda + 1 < \bar{p}$ *where, for notational convenience, we define*

$$R_0(1; [0, 1], Q_\alpha, f_\lambda) = Q_\alpha f_\lambda . \tag{2.21}$$

Proof. Unless both $\lambda < 0$ and $\alpha = 0$, it follows from (2.3) and (2.13)

$$\begin{aligned} Q_\alpha^{(m)} f_\lambda - If_\lambda &= \frac{1}{m} \sum_{j=0}^{m-1} \left(\frac{j+\alpha}{m}\right)^\lambda - \int_0^1 x^\lambda \, dx \\ &= \frac{1}{m^{\lambda+1}} \sum_{j=0}^{m-1} \left((j+\alpha)^\lambda - \int_j^{j+1} x^\lambda \, dx\right). \end{aligned} \tag{2.22}$$

Each term in the summation over j represents the error functional for the one-point rule Q_α over the interval $(j, j+1)$; so except for the $j = 0$ term, the result (2.4) with $m = 1$ may be used. Since $h_p(\alpha, t)$ is periodic in t, one obtains

$$\begin{aligned} Q_\alpha^{(m)} f_\lambda - If_\lambda = &\frac{1}{m^{\lambda+1}} \left(\alpha^\lambda - \int_0^1 f_\lambda(t) \, dt\right) \\ &+ \frac{1}{m^{\lambda+1}} \left(\sum_{s=1}^{p-1} c_s(\alpha) \int_1^m f_\lambda^{(s)}(t) \, dt + \int_1^m h_p(\alpha, t) f_\lambda^{(p)}(t) \, dt\right). \end{aligned} \tag{2.23}$$

To establish the theorem, one replaces the integrals having upper limit m using (2.14) and (2.15) above. Collecting together the terms gives a result of the stated form. It gives also the coefficients as written in (2.18)–(2.20) with $\bar{s} = 0$ and $\bar{p} = p$.

To establish the more general form of (2.20), we note that

$$R_p(m; [0, 1], Q_\alpha, f_\lambda) = m^{-p} B_p([0, 1], Q_\alpha, f_\lambda) + R_{p+1}(m; [0, 1], Q_\alpha, f_\lambda), \quad p \neq [\lambda + 1] \tag{2.24}$$

for $p \leq \lambda$ and $p > \lambda + 1$. For $p > \lambda + 1$, this follows from (2.17) by taking the difference between the formula as written and the formula written with p replaced by $p + 1$. For $p \leq \lambda$, (2.24) follows in the same way from (2.8). But note that this is not valid for $p = [\lambda + 1]$ unless λ is an integer. Using (2.24) in (2.20) with $\bar{s} = 0$ and $\bar{p} = p$, we may extend the result to any values of $\bar{s}$, $\bar{p}$ satisfying $0 \leq \bar{s} < \lambda + 1 < \bar{p}$. This condition is critical. If one sets $\bar{s} < \bar{p} < \lambda + 1$ or $\lambda + 1 < \bar{s} < \bar{p}$ the right hand side of (2.20) reduces to zero. □

We note that in the statement of Theorem 2.4 we have restricted p so that $p > \lambda + 1$. When $p < \lambda + 1$ the corresponding formula is (2.4) since in this case the derivatives of order p or less of $f_\lambda(x)$ are integrable over $[0, 1]$. When λ is an integer, Theorem 2.4 reduces to a special case of Theorem 2.1, many explicit terms dropping out due to the vanishing of derivatives of order $\lambda + 1$ or greater.

The corresponding expansion for a general function having this singularity follows by taking linear superpositions of the results in Theorems 2.1 and 2.4. We find:

Theorem 2.5. *Let* $F_{\lambda,0}(x) = f_\lambda(x) g(x) = x^\lambda g(x)$ *with* $\lambda > -1$ *where* $g(x)$ *and its first* $[p - \lambda]$ *derivatives are integrable in* $[0, 1]$ *and* $p \geq 1$. *Then*

$$Q_\alpha^{(m)}[0, 1]F_{\lambda,0} = \sum_{s=0}^{p-1} \frac{B_s([0, 1], Q_\alpha, F_{\lambda,0})}{m^s}$$

$$+ \sum_{t=0}^{[p-\lambda]-1} \frac{E_{\lambda+t+1}([0, 1], Q_\alpha, F_{\lambda,0})}{m^{\lambda+t+1}} + R_p(m; [0, 1], Q_\alpha, F_{\lambda,0}) \quad (2.26)$$

where coefficients B_s *and* $E_{\lambda+t+1}$ *are dependent of* m *and* $R_p = O(m^{-p})$.

Proof. We define a subtraction function

$$\phi_t(x) = \sum_{l=0}^{t-1} C_{\lambda+l} x^{\lambda+l}, \qquad C_{\lambda+1} = g^{(l)}(0)/l!. \quad (2.27)$$

The function

$$F_{\lambda,0,p}(x) = F_{\lambda,0}(x) - \phi_{[p-\lambda]}(x) \quad (2.28)$$

is by construction one whose first $p-1$ derivatives at $x=0$ are zero and whose pth derivative is integrable. Consequently, we may set

$$Q_\alpha^{(m)} F_{\lambda,0} = Q_\alpha^{(m)} F_{\lambda,0,p} + Q_\alpha^{(m)} \phi_{[p-\lambda]} \quad (2.29)$$

and use Theorem 2.1 to expand the first term on the right. In view of (2.27) the second term on the right is the sum of $[p-\lambda]$ terms to each of which the expansion of Theorem 2.4 may be applied. Collecting together all these expansions, we find after rearrangement an expansion of type (2.26) so establishing the theorem. □

This procedure provides integral representations for the coefficients. For example,

$$\begin{aligned} &R_p(m; [0, 1], Q_\alpha, F_{\lambda,0}) \\ &= R_p(m; [0, 1], Q_\alpha, F_{\lambda,0,p}) + \sum_{l=0}^{[p-\lambda]-1} C_{\lambda+l} R_p(m; [0, 1], Q_\alpha, f_{\lambda+l}) \\ &= \frac{1}{m^p} \int_0^1 h(\alpha, mt) F_{\lambda,0,p}^{(p)}(t)\, dt + \frac{1}{m^p} \sum_{l=0}^{[p-\lambda]-1} C_{\lambda+l} \int_{a_{p-\lambda-l-1}}^1 h(\alpha, mt) f_{\lambda+l}^{(p)}(t)\, dt. \end{aligned} \quad (2.30)$$

In these integrals, the lower limit is 0 or ∞ according as $p - \lambda - l - 1 \gtrless 0$. Collecting terms having the same integration interval together, and using (2.27) and (2.28), we find

$$R_p(m; [0, 1], Q_\alpha, F_{\lambda,0}) = \frac{1}{m^p} \int_0^1 h(\alpha, mt)(F_{\lambda,0}(t) - \phi_{[p-\lambda]}(t))^{(p)}\, dt$$

$$+ \frac{1}{m^p} \int_\infty^1 h(\alpha, mt) \phi_{[p-\lambda]}^{(p)}(t)\, dt. \quad (2.31)$$

A similar calculation gives

$$B_s([0, 1], Q_\alpha, F_{\lambda,0}) = c_s(\alpha)\left[\int_0^1 (F_{\lambda,0}(t) - \phi_{[s-\lambda]}(t))^{(s)}\, dt + \int_\infty^1 \phi_{[s-\lambda]}^{(s)}(t)\, dt\right]. \quad (2.32)$$

The final theorems of this section will deal with an integrand function having algebraic singularities at both ends of the integration interval. To this end we extend our notation and define

$$f_{\lambda,\mu}(x) = x^{\lambda}(1-x)^{\mu}\,, \quad \lambda, \mu > -1\,.$$

Our first result is somewhat trivial.

Theorem 2.6. *Let $f_{0,\mu}(x) = (1-x)^{\mu}$ where $\mu > -1$. Let $Q_{\alpha}^{(m)} f_{0,\mu}$ be finite. Then*

$$Q_{\alpha}^{(m)} f_{0,\mu} = \frac{E_{\mu+1}([0,1], Q_{\alpha}, f_{0,\mu})}{m^{\mu+1}} + \sum_{s=0}^{p-1} \frac{B_s([0,1]\, Q_{\alpha}, f_{0,\mu})}{m^s}$$
$$+ R_p(m; [0,1]; Q_{\alpha}, f_{0,\mu})\,, \quad p \geqslant \mu + 1\,, \tag{2.33}$$

where $E_{\mu+1}$ and B_s are independent of m and $R_p = \mathrm{O}(m^{-p})$.

This is simply a reflection about $x = \frac{1}{2}$ of Theorem 2.4. Of subsequent interest is the representation of the coefficients, which may be derived directly from those following Theorem 2.8. We note that

$$Q_{\alpha}^{(m)} f_{0,\mu} = Q_{1-\alpha}^{(m)} f_{\mu,0}\,, \tag{2.34}$$

$$h_s^{[n]}(\alpha, t) = (-1)^s h_s^{[n]}(1-\alpha, 1-t)\,, \quad n = 0, 1\,. \tag{2.35}$$

Using these we find

$$B_s([0,1], Q_{\alpha}, f_{0,\mu}) = c_s(\alpha) \int_0^{1-a_{s-\mu-1}} f_{0,\mu}^{(s)}(x)\,\mathrm{d}x\,, \quad s = 0, 1, 2, \ldots, \tag{2.36}$$

$$R_s(m; [0,1], Q_{\alpha}, f_{0,\mu}) = \frac{1}{m^s} \int_0^{1-a_{s-\mu-1}} h_s(\alpha, mt) f_{0,\mu}^{(s)}(t)\,\mathrm{d}t\,, \quad s = 1, 2, \ldots \tag{2.37}$$

where a_{ν} is as defined in (2.16) and $E_{\mu+1}([0,1], Q_{\alpha}, f_{0,\mu})$ is defined in terms of these as in (2.20).

In nearly all the expressions we derive subsequently, the integral representations of the coefficients are more useful in the development than any simpler expressions. However, in the next theorem, we need some alternate expressions. We collect these here for future reference.

Lemma 2.7. *When $s \geqslant 1$*

$$B_s([0,1], Q_{\alpha}, G) = c_s(\alpha)(G^{(s-1)}(1) - G^{(s-1)}(0))\,,$$
$$B_s([0,1], Q_{\alpha}, f_{\lambda,0}) = c_s(\alpha) f_{\lambda,0}^{(s-1)}(1)\,, \quad \lambda \neq \text{integer}\,,$$
$$B_s([0,1], Q_{\alpha}, f_{0,\mu}) = -c_s(\alpha) f_{0,\mu}^{(s-1)}(0)\,, \quad \mu \neq \text{integer}\,,$$
$$B_s([0,1], Q_{\alpha}, F_{\lambda,0}) = c_s(\alpha) F_{\lambda,0}^{(s-1)}(0)\,,$$
$$E_{\lambda+1}([0,1], Q_{\alpha}, f_{\lambda}) = \zeta(-\lambda, \alpha)\,, \quad \lambda \neq \text{integer}\,. \tag{2.38}$$

The integral representations from which these may be derived are (2.9), (2.18), (2.36), (2.32) and (2.20), respectively. The final result is established in the Appendix.

We now treat the function

$$F_{\lambda,\mu}(x) = x^{\lambda}(1-x)^{\mu}g(x) \tag{2.39}$$

where λ, μ are not integers and $g(x)$ has integrable derivatives of order $\max([p-\lambda], [p-\mu])$.

We define two subtraction functions, these involving truncated Taylor expansions about each end. Thus

$$\phi_t(x) = C_\lambda x^\lambda + C_{\lambda+1}x^{\lambda+1} + \cdots + C_{\lambda+t-1}x^{\lambda+t-1}, \tag{2.40}$$

$$\psi_t(x) = \tilde{C}_\mu(1-x)^\mu + \tilde{C}_{\mu+1}(1-x)^{\mu+1} + \cdots + \tilde{C}_{\mu+t-1}(1-x)^{\mu+t+1}. \tag{2.41}$$

The coefficients are

$$C_{\lambda+l} = \frac{1}{l!}\frac{\mathrm{d}^l}{\mathrm{d}x^l}[(1-x)^\mu g(x)]_{x=0}, \qquad \tilde{C}_{\mu+l} = \frac{(-1)^l}{l!}\frac{\mathrm{d}^l}{\mathrm{d}x^l}[x^\lambda g(x)]_{x=1}. \tag{2.42}$$

We define

$$F_{\lambda,\mu,p}(x) = F_{\lambda,\mu}(x) - \phi_{[p-\lambda]}(x) - \psi_{[p-\mu]}(x) \tag{2.43}$$

and note that the first $(p-1)$ derivatives of this function are continuous both at $x=0$ and at $x=1$ and so its pth derivative is integrable. Using the fact that μ is non-integer, and that the first $p-1$ derivatives of $F_{\lambda,\mu}(x) - \phi_{[p-\lambda]}(x)$ are zero at $x=0$ we find from (2.43) that

$$F^{(s)}_{\lambda,\mu,p}(0) + \psi^{(s)}_{[p-\mu]}(0) = 0, \quad s = 0, 1, \ldots, p-1. \tag{2.44}$$

Similarly, since λ is not an integer

$$F^{(s)}_{\lambda,\mu,p}(1) + \phi^{(s)}_{[p-\lambda]}(1) = 0, \quad s = 0, 1, \ldots, p-1. \tag{2.45}$$

Theorem 2.8. *Let $F_{\lambda,\mu}(x) = x^\lambda(1-x)^\mu g(x)$ where λ, μ are not integers and $g(x)$ has integrable derivatives of order* $\max([p-\lambda], [p-\mu])$. *Let $Q^{(m)}_\alpha F_{\lambda,\mu}$ be finite; then*

$$\begin{aligned} Q^{(m)}_\alpha F_{\lambda,\mu} = IF_{\lambda,\mu} &+ \sum_{t=0}^{[p-\lambda]-1} \frac{E_{\lambda+t+1}([0,1], Q_\alpha, F_{\lambda,\mu})}{m^{\lambda+t+1}} \\ &+ \sum_{t=0}^{[p-\mu]-2} \frac{E_{\mu+t+1}([0,1], Q_\alpha, F_{\lambda,\mu})}{m^{\mu+t+1}} + R_p(m; [0,1], Q_\alpha, F_{\lambda,\mu}), \quad p > 1, \end{aligned} \tag{2.46}$$

where $E_{\lambda+t+1}$ and $E_{\mu+t+1}$ are independent of m and $R_p = \mathrm{O}(m^{-p})$.

Proof. For $m > 1$, splitting the interval into two parts and applying Theorem 2.5 to each part separately establishes this form, but with additional terms of the form $\Sigma_{s=1}^{p-1} B_s/m^s$. To establish the theorem as stated, we have to show that these terms disappear. In view of definition (2.43) we have

$$Q^{(m)}_\alpha F_{\lambda,\mu} = Q^{(m)}_\alpha F_{\lambda,\mu,t} + Q^{(m)}_\alpha \phi_{[t-\lambda]} + Q^{(m)}_\alpha \psi_{[t-\mu]}. \tag{2.47}$$

Since $F_{\lambda,\mu,t}$ has integrable derivatives of order p, we apply (2.4) to evaluate the first term on the right. Since $\phi_{[p-\lambda]}$ is a sum (2.40) of elements $f_{\lambda+j}$ we may use (2.17) on each element to evaluate the second term on the right. Similarly we use (2.33) for the third term. Collecting together the coefficients of m^{-s} we find

$$B_s([0,1], Q_\alpha, F_{\lambda,\mu}) = B_s([0,1], Q_\alpha, F_{\lambda,\mu,p}) + \sum_{t=0}^{[p-\lambda]-1} C_{\lambda+t} B_s([0,1], Q_\alpha, f_{\lambda+t,0})$$
$$+ \sum_{t=0}^{[p-\mu]-1} \tilde{C}_{\mu+t} B_s([0,1], Q_\alpha, f_{0,\mu+t}) \quad s = 0, 1, \ldots . \tag{2.48}$$

Using the expressions in Lemma 2.7 to simplify this, we find

$$B_s([0,1], Q_\alpha, F_{\lambda,\mu}) = c_s(\alpha)\Big[(F^{(s-1)}_{\lambda,\mu,p}(1) - F^{(s-1)}_{\lambda,\mu,p}(0)) + \sum_{t=0}^{[p-\lambda]-1} C_{\lambda+t} f^{(s-1)}_{\lambda+t,0}(1)$$
$$- \sum_{t=0}^{[p-\mu]-1} \tilde{C}_{\mu+t} f^{(s-1)}_{0,\mu+t}(0)\Big], \quad s = 1, 2, \ldots . \tag{2.49}$$

In view of identities (2.44) and (2.45), the expression in square brackets is identically zero and so $B_s = 0$ for $s \geq 1$. The theorem now follows by identifying the nature of the contributions from each term of (2.47). □

This procedure provides integral representations for the coefficients in (2.46). Thus the remainder term is the sum of the three remainder terms corresponding to the three terms in (2.47). This sum resembles that in (2.48). Using (2.10), (2.19) and (2.37), we find

$$R_p(m; [0,1], Q_\alpha, F_{\lambda,\mu}) = m^{-p} \int_0^1 h_p(\alpha, mt) F^{(p)}_{\lambda,\mu,p}(t)\, dt$$
$$+ \sum_{s=0}^{[p-\lambda]-1} C_{\lambda+s} m^{-p} \int_{a_{p-\lambda-1}}^1 h_p(\alpha, mx) f^{(p)}_{\lambda+s,0}(x)\, dx$$
$$+ \sum_{s=0}^{[p-\mu]-1} \tilde{C}_{\mu+s} m^{-p} \int_0^{1-a_{p-\mu-s-1}} h_p(\alpha, mt) f^{(p)}_{0,\mu+s}(x)\, dx \tag{2.50}$$
$$= m^{-p}\Big\{\int_0^1 h_p(\alpha, mt)(F_{\lambda,\mu}(t) - \phi_{[p-\lambda]}(t) - \psi_{[p-\mu]}(t))^{(p)}\, dt$$
$$+ \int_\infty^1 h_p(\alpha, mt)\phi^{(p)}_{[p-\lambda]}(t)\, dt + \int_0^{-\infty} h_p(\alpha, mt)\psi^{(p)}_{[p-\mu]}(t)\, dt\Big\}$$

and

$$E_{\lambda+t+1}([0,1], Q_\alpha, F_{\lambda,\mu}) = C_{\lambda+t} E_{\lambda+t+1}([0,1], Q_\alpha, f_{\lambda+t,0}),$$
$$E_{\mu+t+1}([0,1], Q_\alpha, F_{\lambda,\mu}) = \tilde{C}_{\mu+t} E_{\mu+t+1}([0,1], Q_\alpha, f_{0,\mu+t}) \tag{2.51}$$

where $C_{\lambda+t}$ and $\tilde{C}_{\mu+t}$ are defined by (2.41) and the coefficients on the right are given by (2.20) and its counterpart.

3. Two-dimensional integrands with one line singularity

In this section we shall be dealing with integration over the square

$$H_2\colon\ 0 \leqslant x,\ y \leqslant 1\,.$$

In all subsequent sections, we shall treat only the one-point rule

$$Q_{\alpha,\beta}G = G(\alpha,\ \beta)$$

and its m^2-copy

$$Q^{(m)}_{\alpha,\beta}G = \frac{1}{m^2}\sum_{j=0}^{m-1}\sum_{k=0}^{m-1} G\left(\frac{\alpha+j}{m},\ \frac{\beta+k}{m}\right)$$

and we shall suppress explicit reference to this rule in the formulas for the coefficients. We shall be particularly interested in obtaining explicit integral representations for the remainder term as these are needed to construct the coefficients in subsequent more sophisticated expansions. We draw attention to this because some of the results of this section may be derived in an easier manner if one only requires order estimates for the remainder term.

In this section we shall derive the two-dimensional Euler–Maclaurin summation formula for a function $\Gamma_\lambda(x,\ y) = x^\lambda G(x,\ y)$ where $G(x,\ y)$ has early integrable derivatives. In the process we shall treat first $F_\lambda(x,\ y) = x^\lambda G(y)$ and then $G(x,\ y)$ and construct the result for $\Gamma_\lambda(x,\ y)$ from the two previous results.

Lyness and McHugh [4], described a formalism to deal with an analytic function $G(x,\ y)$ which provides an integral representation for the remainder term. That formalism may not be directly used for a function such as $x^\lambda G(x,\ y)$ mainly because some of the integrals involved in (2.18) have limits $(0, 1)$ and others $(1, \infty)$. Nevertheless, the underlying algebra may be used for a product function $x^\lambda G(y)$. In [4] the quantities $D^{[n]}_w$, $\delta^{[n]}_w$ stand for differential operators. Here we employ numbers D^n_w, which correspond to $I^{[n]}D^{[n]}_w F$. The description given here is self explanatory.

Let us denote an expansion of D^n_0 by

$$D^n_0 = \delta^n_0 + \delta^n_1 + \cdots + \delta^n_{p-1} + D^n_p\,, \quad p = 1, 2, \ldots\,. \tag{3.1}$$

The terms in the expansion are δ^n_j and the remainder term is D^n_p. Any of the expansions in Section 2 could be expressed in these terms. We take two independent expansions of this type (distinguished by superscripts 1 and 2) and consider an expansion for $D^1_0 D^2_0$. Let

$$\sigma_s = \sum_{k=0}^{s} \delta^1_k \delta^2_{s-k}\,. \tag{3.2}$$

Using only the defining identities

$$D^n_j = \delta^n_j + D^n_{j+1}\,, \qquad j = 0, 1, \ldots, p-1\,, \quad n = 1, 2 \tag{3.3}$$

it is possible to establish the expansion

$$D^1_0 D^2_0 = \sum_{s=0}^{p-1} \sigma_s + \sum_{j=0}^{p} X^1_j X^2_{p-j}\,, \quad p \geqslant 1\,, \tag{3.4}$$

where, in the remainder term, X_0^n stands for δ_0^n, X_j^n stands for either δ_j^n or D_j^n, and in each product $X_j^1 X_{p-j}^2$ at least one factor X stands for D. The proof in this two-dimensional context is straightforward. In [4], the corresponding n-dimensional result is derived. An example of (3.4) with $p=3$ is

$$\begin{aligned} D_0^1 D_0^2 &= \delta_0^1\delta_0^2 + \delta_0^1\delta_1^2 + \delta_1^1\delta_0^2 + \delta_0^1\delta_2^2 + \delta_1^1\delta_1^2 + \delta_2^1\delta_0^2 \\ &\quad + \delta_0^1 D_3^2 + \delta_1^1 D_2^2 + D_2^1 D_1^2 + D_3^1 \delta_0^2 . \end{aligned} \tag{3.5}$$

Note the lack of symmetry between δ and D in the final four terms. For subsequent notational convenience, we restate result (3.4) in the following form.

Definition 3.1. For a given $p>1$, there exist a set of *remainder term index pairs* $[\theta_{j,p}^1, \theta_{p-j,p}^2]$, $j=0,1,\ldots,p$, each of which takes the value $[0,1]$, $[0,0]$ or $[1,0]$, in terms of which

$$D_0^1 D_0^2 = \sum_{s=0}^{p-1} \sigma_s + \sum_{j=0}^{p} (\theta_{j,p}^1 \delta_j^1 + (1-\theta_{j,p}^1) D_j^1)(\theta_{p-j,p}^2 \delta_{p-j}^2 + (1-\theta_{p-j,p}^2) D_{p-j}^2) . \tag{3.7}$$

Note that

$$\theta_{0,p}^1 = \theta_{0,p}^2 = 1 , \qquad \theta_{j,p}^1 + \theta_{p-j,p}^2 \leqslant 1 . \tag{3.8}$$

For a given p, there are several choices for this set of index pairs. One choice is

$$(\theta_{j,k+j}^1, \theta_{k,k+j}^2) = \begin{cases} (0,1) & j-k \geqslant 2 , \\ (0,0) & j-k = 1,0 , \\ (1,0) & j-k \leqslant -1 . \end{cases} \tag{3.9}$$

This is the one illustrated in (3.4).

We now apply the formalism to obtain the Euler–Maclaurin expansion for $Q_{\alpha,\beta}F_\lambda - IF_\lambda$ where

$$F_\lambda(x,y) = x^\lambda G(y) . \tag{3.10}$$

We define

$$\begin{aligned} &D_1^0 = Q_\alpha f_\lambda , \\ &D_p^1 = R_p(m; [0,1], Q_\alpha, f_\lambda) , \quad p \geqslant 1 , \\ &\delta_s^1 = m^{-s} B_s([0,1], Q_\alpha, f_\lambda) , \quad s \leqslant [\lambda] \text{ and } s \geqslant [\lambda+2] , \\ &\delta_s^1 = m^{-s} B_s([0,1], Q_\alpha, f_\lambda) + m^{-\lambda-1} E_{\lambda+1}([0,1], Q_\alpha, f_\lambda) , \quad s = [\lambda+1] ; \end{aligned} \tag{3.11}$$

$$\begin{aligned} &D_0^2 = Q_\beta G , \\ &D_p^2 = R_p(m; [0,1], Q_\beta, G) , \quad p \geqslant 1 , \\ &\delta_s^2 = m^{-s} B_s([0,1], Q_\beta, G) , \quad s \geqslant 0 , \end{aligned} \tag{3.12}$$

so that (3.1) with $n=1$ coincides with expansion (2.17) and with $n=2$ coincides with expansion (2.4). Direct application of (3.7) gives the following theorem.

Theorem 3.2. *Let $F_\lambda(x, y) = x^\lambda G(y)$ where $G(y)$ and its first p derivatives are integrable. Then*

$$Q^{(m)}_{\alpha,\beta}(H_2)F_\lambda = \sum_{s=0}^{p-1} \frac{B_s(H_2, F_\lambda)}{m^s} + \sum_{t=0}^{[p-\lambda]-1} \frac{E_{\lambda+1+t}(H_2, F_\lambda)}{m^{\lambda+1+t}} + R_p(m; H_2, F_\lambda) \tag{3.13}$$

where the coefficients B_s and $E_{\lambda+1+t}$ are independent of m and $R_p = \mathrm{O}(m^{-p})$.

Expressions for these coefficients are given in (3.14)–(3.18) below and integral representations in (3.22)–(3.24) below.

Proof. The left hand side of (3.13) is simply $D^1_0 D^2_0$. We expand $D^1_0 D^2_0$ using (3.7) and re-express the series using (3.11) and (3.12). Collecting together the terms gives the right hand side of (3.13) with

$$B_s(H_2, F_\lambda) = \sum_{k=0}^{s} B_k([0, 1], Q_\alpha, f_\lambda)B_{s-k}([0, 1], Q_\beta, G), \tag{3.14}$$

$$E_{\lambda+1+t}(H_2, F_\lambda) = E_{\lambda+1}([0, 1], Q_\alpha, f_\lambda)B_t([0, 1], Q_\beta, G), \tag{3.15}$$

$$\begin{aligned} R^{(1)}_p&(m; H_2, F_\lambda) \\ &= \sum_{j=0}^{p} (m^{-j}\theta^1_{j,p}B_j([0, 1], Q_\alpha, f_\lambda) + (1-\theta^1_{j,p})R_j(m; [0, 1], Q_\alpha, f_\lambda)) \\ &\quad \times (m^{j-p}\theta^2_{p-j,p}B_{p-j}([0, 1], Q_\beta, G) + (1-\theta^2_{p-j,p})R_{p-j}(m; [0, 1], Q_\beta, G)), \end{aligned} \tag{3.16}$$

$$R^{(2)}_p(m; H_2, F_\lambda) = m^{-\lambda-1}\theta^1_{[\lambda+1],p}E_{\lambda+1}([0, 1], Q_\alpha, f_\lambda)R_{p-[\lambda+1]}(m; [0, 1], Q_\beta, G), \tag{3.17}$$

$$R_p(m; H_2, F_\lambda) = R^{(1)}_p(m; H_2, F_\lambda) + R^{(2)}_p(m; H_2, F_\lambda). \tag{3.18}$$

The quantities on the right hand sides of these equations are defined in (2.9), (2.10), (2.18), (2.19) and (2.20). Clearly, B_s and $E_{\lambda+1+t}$ are independent of m. The remainder term R_p has been divided into two components, one of which is $\mathrm{O}(m^{-p})$ and the other $\mathrm{O}(m^{-p-\{\lambda\}})$ where $\{\lambda\}$ is the fractional part of λ, i.e. $\lambda = [\lambda] + \{\lambda\}$. The indices $\theta^n_{k,p}$ may be set to 1 or 0 according to (3.9). □

Each element of (3.14) to (3.18) is a sum of products of terms each of which has an integral representation given in Section 2. Consequently, we may form an integral representation for each of these terms. Before doing this, we shall introduce some concise notation, (3.19)–(3.21) below, in terms of which the coefficients are expressed in (3.22)–(3.24).

Definition 3.3.

$$t^{[\theta^1,\theta^2]}_{j,k}(m; F)^{b\ d}_{a\ c} = \int_a^b \mathrm{d}x \int_c^d \mathrm{d}y\, (h^{[\theta^1]}_j(\alpha, mx)h^{[\theta^2]}_k(\beta, my))(F^{(j,k)}(x, y)), \quad \theta^n = 0, 1. \tag{3.19}$$

(We recall from (2.5) that $h^{[1]}_j(\alpha, mx) = c_j(\alpha)$ and $h^{[0]}_j(\alpha, mx) = h_j(\alpha, mx)$.) Here a, b, c and d may take any values which define integration limits.

In nearly all contexts, the limits a, b, c, d will take on predictable values, namely $b = d = 1$ and a, $c = 0$, ∞ or 2. For this reason we are able to suppress the values of a, b, c, d. When this is done, the reader should assume default values as follows.

Default Values in (*3.19*): $b = d = 1$; $a = 0$, unless this makes the integral diverge, in which case $a = \infty$ unless this also makes the integral diverge, in which case $a = 2$. c is assigned by the same method as a.

For example, with $F_\lambda(x, y) = x^\lambda G(y)$,

$$t_{j,k}^{[1,1]}(m, F_\lambda) = \int_a^1 \int_0^1 c_j(\alpha) c_k(\beta) F_\lambda^{(j,k)}(x, y)\,\mathrm{d}x\,\mathrm{d}y \tag{3.20}$$

with $a = a_{j-\lambda-1}$. The lower limits are those which ensure the integral exists. A second minor notational abbreviation is also employed. The remainder term indices $[\theta^1, \theta^2]$ are replaced by $[\cdot\,\cdot]$ when their values are obvious from the context. Thus, in

$$t_{j,k}^{[\cdot\,\cdot]}(m, F)_{a\ c}^{b\ d}$$

the superscript $[\cdot\,\cdot]$ stands for $[\theta^1_{j,j+k}, \theta^2_{k,j+k}]$ as defined in (3.9).

A second complicated definition will be helpful.

$$U_k^{[\theta^2]}(m, F_\lambda)_c^d = t_{\bar{s},k}^{[0,\theta^2]}(m, F_\lambda)_{0\ c}^{1\ d} - \sum_{s=\bar{s}}^{\bar{p}-1} t_{s,k}^{[1,\theta^2]}(m, F_\lambda)_{a_{s-\lambda-1}\ c}^{1\qquad d} - t_{\bar{p},k}^{[0,\theta^2]}(m, F_\lambda)_{\infty\ c}^{1\ d} \tag{3.21}$$

where, as before $0 \leqslant \bar{s} < \lambda + 1 < \bar{p}$. Here $a = a_{s-\lambda-1}$ is the value which makes the integral converge.

Besides enabling us to express results in relatively compact form, the use of this notation facilitates subsequent manipulation.

For subsequent convenience, we define

$$V_k^{[\theta^1]}(m, F_\mu)_a^b = t_{k,\bar{s}}^{[\theta^1,0]}(m, F_\mu)_{a\ 0}^{b\ 1} - \sum_{s=\bar{s}}^{\bar{p}-1} t_{k,s}^{[\theta^1,1]}(m, F_\mu)_{a\ c}^{b\ 1} - t_{k,\bar{p}}^{[\theta^1,0]}(m, F_\mu)_{a\ \infty}^{b\ 1} \tag{3.21a}$$

where $0 \leqslant \bar{s} < \mu + 1 < \rho$ and $c = a_{s-\mu-1}$. This coefficient is used in the expansion of a function of the form $F_\mu(x, y) = y^\mu G(x)$.

Substituting the expressions in Section 2 for the coefficients on the right hand side of (3.14)–(3.17) and simplifying the resulting expressions using (3.19)–(3.21a) we find

$$B_s(H_2, F_\lambda) = \sum_{k=0}^{s} t_{k,s-k}^{[1,1]}(1, F_\lambda)\,, \tag{3.22}$$

$$E_{\lambda+1+t}(H_2, F_\lambda) = U_t^{[1]}(1, F_\lambda)\,, \tag{3.23}$$

$$R_p(m; H_2, F_\lambda) = \frac{1}{m^p} \sum_{j=0}^{p} t_{j,p-j}^{[\cdot\,\cdot]}(m, F_\lambda) + \frac{\theta^1_{[\lambda+1],p}}{m^{p+\{\lambda\}}}\, U_{p-[\lambda+1]}^{[0]}(m, F_\lambda) \tag{3.24}$$

the coefficients on the right being defined in (3.19)–(3.21a). Here $\{\lambda\} = \lambda - [\lambda]$ is the fractional part of λ.

The following theorem is a minor modification of one derived in [4].

Theorem 3.4. *Let $G(x, y)$ and its partial derivatives of order p or less be integrable over H_2. Then*

$$Q_{\alpha,\beta}(H_2)G = \sum_{s=0}^{p-1} \frac{B_s(H_2, G)}{m^s} + R_p(m; H_2, G) \tag{3.25}$$

where integral representations of the coefficients are

$$B_s(H_2, G) = \sum_{k=0}^{s} t^{[1,1]}_{k,s-k}(1, G), \tag{3.26}$$

$$R_p(m; H_2, G) = \frac{1}{m^p} \sum_{j=0}^{p} t^{[\cdot\,\cdot]}_{j,p-j}(m, G). \tag{3.27}$$

The coefficients on the right are defined in (3.19)–(3.20). Note that here all the lower limits are zero, making this a somewhat straightforward result. We now establish the important theorem of this section.

Theorem 3.5. *Let $\Gamma_\lambda(x, y) = x^\lambda G(x, y)$ where $\lambda > -1$ and the derivatives $G^{(r,s)}(x, y)$ are integrable for $r \leqslant [p - \lambda]$ and $s \leqslant p$, then*

$$Q_{\alpha,\beta}(H_2)\Gamma_\lambda = \sum_{s=0}^{p-1} \frac{B_s(H_2, \Gamma_\lambda)}{m^s} + \sum_{t=0}^{[p-\lambda]-1} \frac{E_{\lambda+1+t}(H_2, \Gamma_\lambda)}{m^{\lambda+1+t}} + R_p(m; H_2, \Gamma_\lambda) \tag{3.28}$$

where B_s and $E_{\lambda+1+t}$ are independent of m and $R_p = \mathrm{O}(m^{-p})$.

Proof. Here, as in the proof of the similar one-dimensional Theorem 2.5 we use a subtraction function to express $\Gamma_\lambda(x, y)$ in terms of functions whose expansion we have available. Let

$$\phi_t(x, y) = \sum_{l=0}^{t-1} x^{\lambda+l} G^{(l,0)}(0, y)/l! = \sum_{l=0}^{t-1} F_{\lambda+l}(x, y), \tag{3.29}$$

and let

$$\Gamma_{\lambda,w}(x, y) = \Gamma_\lambda(x, y) - \phi_w(x, y) \tag{3.30}$$

with

$$w = p - [\lambda + 1] = [p - \lambda].$$

$\phi_w(x, y)$ is a sum of functions each of which is of form (3.10) while $\Gamma_{\lambda,w}$ and its partial derivatives of order p or less are integrable over H_2. Thus we may set

$$Q^{(m)}_{\alpha,\beta}\Gamma_\lambda = Q^{(m)}_{\alpha,p}\Gamma_{\lambda,w} + Q^{(m)}_{\alpha,\beta} \sum_{l=0}^{w-1} F_{\lambda+l} \tag{3.31}$$

and apply Theorem 3.4 to the first term on the right and Theorem 3.2 to each of the terms in the sum over l. This gives (3.28) with

$$B_s(H_2, \Gamma_\lambda) = \sum_{l=0}^{w-1} B_s(H_2, F_{\lambda+l}) + B_s(H_2, \Gamma_{\lambda,w}), \tag{3.32}$$

$$E_{\lambda+1+t}(H_2, \Gamma_\lambda) = \sum_{l=0}^{t} E_{\lambda+1+t}(H_2, F_{\lambda+l}), \tag{3.33}$$

$$R_p(m; H_2, \Gamma_\lambda) = \sum_{l=0}^{w-1} R_p(m; H_2, F_{\lambda+l}) + R_p(m; H_2, \Gamma_{\lambda,w}) \tag{3.34}$$

which clearly satisfy the conditions of the theorem.

We next employ (3.22)–(3.24) and (3.26)–(3.27) to obtain integral representations for these coefficients. Direct application of (3.22) and (3.26) reduces (3.32) to the form

$$B_s(H_2, \Gamma_\lambda) = \sum_{l=0}^{w-1} \sum_{k=0}^{s} t_{k,s-k}^{[1,1]}(1, F_{\lambda+l}) + \sum_{k=0}^{s} t_{k,s-k}^{[1,1]}(1, \Gamma_{\lambda,w}). \tag{3.35}$$

The integration interval in the x direction is $(\infty, 1]$ when $\lambda + l - k < -1$, is $[0, 1]$ when $\lambda + l - k > -1$, and is $[0, 1]$ in the final term. In cases in which the interval of integration is the same, we may invert the summation and integration order. Thus, we may rewrite (3.35) in the form

$$\sum_{k=0}^{s} \left(\sum_{l=0}^{[k-\lambda-1]} t_{k,s-k}^{[1,1]}(1, F_{\lambda+l}) + \sum_{l=[k-\lambda]}^{w-1} t_{k,s-k}^{[1,1]}(1, F_{\lambda+l}) + t_{k,s-k}^{[1,1]}(1, \Gamma_{\lambda,w}) \right).$$

Introducing the subtraction function (3.29), this reduces to the form (3.36) given below. A similar rearrangement may be carried out in the remainder term.

We find

$$B_s(H_2, \Gamma_\lambda) = \sum_{k=0}^{s} t_{k,s-k}^{[1,1]}(1, \phi_{[k-\lambda]})_{\infty\ 0}^{1\ 1} + t_{k,s-k}^{[1,1]}(1, \Gamma_\lambda - \phi_{[k-\lambda]})_{0\ 0}^{1\ 1}, \tag{3.36}$$

$$E_{\lambda+1+r}(H_2, \Gamma_\lambda) = \sum_{l=0}^{t} U_{t-l}^{[1]}(1, F_{\lambda+l})_0^1, \tag{3.37}$$

$$\begin{aligned} R_p(m; H_2, \Gamma_\lambda) = {} & \frac{1}{m^p} \sum_{k=0}^{p} t_{k,p-k}^{[\cdot\ \cdot]}(m, \phi_{[k-\lambda]})_{\infty\ 0}^{1\ 1} + t_{k,p-k}^{[\cdot\ \cdot]}(m, \Gamma_\lambda - \phi_{[k-\lambda]})_{0\ 0}^{1\ 1} \\ & + \frac{1}{m^{p+\{\lambda\}}} \sum_{l=0}^{[p-\lambda]-1} \theta_{[\lambda+l+1],p}^{1} U_{p-l-[\lambda]-1}^{[0]}(m, F_{\lambda+l})_0^1. \end{aligned} \tag{3.38}$$

Alternative expressions for B_s and $E_{\lambda+1+t}$ may be derived by evaluating the integrals in (2.18) and (2.20), i.e.

$$\begin{aligned} B_s([0, 1], Q_\alpha, f_\lambda) &= c_s(\alpha) f_\lambda^{(s-1)}(1) \\ &= -\zeta(1-s, \alpha)\lambda!/((s-1)!(\lambda-s+1)!), \quad \lambda \neq \text{integer}, \end{aligned} \tag{3.39}$$

$$E_{\lambda+1}([0, 1], Q_\alpha, f_\lambda) = \zeta(-\lambda, \alpha), \quad \lambda \neq \text{integer}. \tag{3.40}$$

These leads to

$$B_s(H_2, \Gamma_\lambda) = \sum_{k=0}^{s} c_k(\alpha)c_{s-k}(\beta)(\Gamma_\lambda^{(k-1,s-k-1)}(1,1) - \Gamma_\lambda^{(k-1,s-k-1)}(1,0)) ,$$

$$\lambda \neq \text{integer} , \quad (3.41)$$

$$E_{\lambda+1+t}(H_2, \Gamma_\lambda)$$

$$= \sum_{l=0}^{t} \zeta(-\lambda - l, \alpha)c_{t-l}(\beta) \frac{1}{l!} (G^{(l,t-l-1)}(0,1) - G^{(l,t-l-1)}(0,0)) , \quad \lambda \neq \text{integer} .$$

$$(3.42)$$

Both require proper interpretation as integrals when a superscript is -1. When the second superscript is -1, the pair of terms should be replaced by an integral in y over $[0, 1]$, in a standard manner. In (3.41) when the first superscript is -1, that is $k = 0$, each of the terms $\Gamma_\lambda^{(0,s-1)}(1, y)$ should be separately replaced by an integral in x over $[0, 1]$ of $\Gamma_\lambda^{(0,s-1)}(x, y)$.

4. Ignoring the singularity

The results of this paper apply for all the integrand functions treated here, so long, of course, that the quadrature rule sum $Q_\alpha^{(m)} f$ exists. Generally, this condition coincides with the condition that the integral If exists. However, not always; in some cases an abscissa $(j + \alpha)/m$ may be a point at which the function value is indeterminate. This happens, for example, when $f(x) = x^\lambda$ with $-1 < \lambda < 0$ and $\alpha = 0$. It is generally believed that in practice one may 'ignore' such inconvenient points, i.e. assign $f(0) = 0$. In fact, it may be readily established that this is a proper procedure for the classes of integrand functions treated in this paper. Here all singularities occur on the boundary and so only when α or β take values 0 or 1 does the problem arise. We describe here the adjustment of the theory necessary to cover the case $\alpha = 0$.

We define a modified rule

$$\bar{Q}_0^{(m)} f = \frac{1}{m} \sum_{j=1}^{m-1} f(j/m) . \quad (4.1)$$

When $f(0)$ is defined, this is identical with

$$\bar{Q}_0^{(m)} f = Q_0^{(m)} f - (1/m)f(0) . \quad (4.2)$$

When $f(x) = f_\lambda(x) = x^\lambda$ with $\lambda \neq 0$, the use of the modified rule coincides precisely with using the unmodified rule and 'ignoring the singularity'. (Note $f_\lambda(0) = 0$ for $\lambda > 0$.) Thus, if we wish to modify the theory to allow 'ignoring the singularity' we need only reconstruct the theory for rule (4.1).

In fact, such a reconstruction alters very little. Theorem 2.4 is the point in the theory where modification first becomes necessary. However, so long as λ is non-integer, this theorem and all equations required in its proof remain valid precisely as written when one sets $\alpha = 0$, replaces $Q_0^{(m)} f_\lambda$ by $\bar{Q}_0^{(m)} f_\lambda$ and removes the term $\alpha^\lambda/m^{\lambda+1}$ from the right hand sides of (2.22) and (2.23). The effect of this in the rest of the paper is that all theorems are valid in the context of ignoring the singularity (so long as parameters λ and μ are non-integer).

When $f(x)$ has no singularity at $x=0$ and the modified rule $\bar{Q}_0^{(m)} f$ is used, it ignores a finite function value. To complete the theory for the rule $\bar{Q}_0^{(m)} f$, one has to note that in the modified version of Theorem 2.1, all coefficients except B_1 take their unmodified values. However,

$$B_1([0,1], \bar{Q}_0, G) = B_1([0,1], Q_0, G) - G(0)\,, \tag{4.3}$$

The result is actually needed in the proof of the modification of Theorem 2.8. When $\bar{Q}_0$ replaces Q_0, two of the terms in (2.47) represent 'ignoring finite function values'. However, in view of (2.44), these two terms eliminate each other and the final result is precisely as stated.

5. Concluding remarks

The reader will have noticed that, although the principal results of this paper are asymptotic expansions, in every case an explicit representation of the remainder term is given. No appeal to the theory of asymptotic expansions has been necessary.

The techniques of this paper may be employed to construct expansions of the same nature for integrand functions having algebraic singularities along several of the sides. We have determined some of these. These are

$$f(x, y) = x^{\lambda_1} y^{\lambda_2} (1-x)^{\lambda_3} (1-y)^{\lambda_4} G(x, y)$$

with two of, three of and all four of λ_i non-integer. The expansions are quite predictable, being of the form

$$Q_{\alpha,\beta}^{(m)} f = \sum_{s=0}^{p-1} \frac{B_s}{m^s} + \sum_{i=1}^{4}{}^{*} \sum_{t=0} \frac{E_{\lambda_i+t+1}}{m^{\lambda_i+t+1}} + R_p(m)\,,$$

the asterisk on the sum over i indicating that the sum is restricted to values of i for which λ_i is non-integer. When all four λ_i are non-integer, one finds $B_s = 0$; $s \geqslant 1$. Otherwise, in general, all terms are non-vanishing. In particular, Theorem 2.8 notwithstanding, the B_s terms do not vanish in the case $\lambda_2 = \lambda_4 = 0$, λ_1, λ_3 non-integer.

For integrands having point singularities of the type

$$f(x, y) = (\sqrt{x^2+y^2})^{\rho} G(x, y) \quad \tfrac{1}{2}\rho \text{ non-integer}\,,$$

expansions are given by Lyness [3]. In part 2 of this paper, we shall exploit the results of this part to generalize the results of Lyness to integrand functions having intersecting point and line singularities. These will include

$$f(x, y) = x^{\lambda} y^{\mu} (\sqrt{x^2+y^2})^{\rho} G(x, y)$$

and others like it.

Appendix A. Required properties of the zeta-function

The properties of the Bernoulli polynomials $B_s(x)$ and the Bernoulli functions $\bar{B}_s(x)$ are well known. In the text we have defined

$$c_s(\alpha) = B_s(\alpha)/s!\,, \qquad h_s(\alpha, t) = (B_s(\alpha) - \bar{B}_s(\alpha - t))/s!\,. \tag{A.1}$$

In terms of these, the Euler–Maclaurin expansion (2.4) for the finite interval [0, 1] takes the form described in Theorem 2.1.

A form for the semi infinite interval may be obtained by applying (2.4) with $m = 1$ to each of the intervals (1, 2), (2, 3), (3, 4), . . . and summing the result. This gives

Theorem A.2. *So long as $\phi^{(p)}(t)$ is integrable in the interval* $[1, \infty)$

$$\sum_{j=1}^{\infty} \phi(j + \alpha) = \sum_{s=0}^{p-1} c_s(\alpha) \int_1^{\infty} \phi^{(s)}(x)\,\mathrm{d}x + \int_1^{\infty} h_p(\alpha, t)\phi^{(p)}(t)\,\mathrm{d}t\,. \tag{A.2}$$

We shall use this later.

The properties of the (Hurwitz) zeta function are less well known. This is conventionally defined (for $\lambda < -1$) by

$$\zeta(-\lambda, \alpha) = \alpha^{\lambda} + (\alpha + 1)^{\lambda} + (\alpha + 2)^{\lambda} + \cdots, \qquad \alpha > 0\,, \quad \lambda < -1\,. \tag{A.3}$$

By reexpressing this as a contour integral, it may be shown that this is an analytic function in λ, having a single pole at $\lambda = -1$; see for example [6, p. 266]. Thus its analytic continuation for $\lambda > -1$ exists. To obtain the result we need in (2.38) we set $\phi(x) = x^{\lambda}$ and $p > \lambda + 1$ in (A.2). Direct evaluation of the integrals gives

$$\zeta(-\lambda, \alpha) = \alpha^{\lambda} - \sum_{s=0}^{p-1} c_s(\alpha) \frac{\lambda!}{(\lambda - s + 1)!} + \int_1^{\infty} h_p(\alpha, t) \frac{\lambda!}{(\lambda - p)!} t^{\lambda - p}\,\mathrm{d}t\,, \quad p > \lambda + 1 \tag{A.4}$$

with the further restriction $\lambda < -1$. However, this restriction may be lifted since each element in equation (A.4) is an analytic function of λ and so by analytic continuation, the equation remains valid for all λ. It is readily verified that, with $\bar{s} = 0$ and $p = \bar{p}$, the right hand side of (2.20) reduces to the right hand side of (A.4), establishing the result that $E_{\lambda+1} = \zeta(-\lambda, \alpha)$. Further, useful results include

$$\zeta(-s + 1, \alpha) = -B_s(\alpha)/s\,, \quad \forall\,\text{integer}\ s \geq 1\,, \tag{A.5}$$

and

$$\zeta(-\lambda, \alpha) = 2\lambda! \sum_{r=1}^{\infty} \frac{\sin[2\pi\alpha r - \pi\lambda/z]}{(2\pi r)^{\lambda+1}}, \qquad \operatorname{Re}\lambda > 0\,. \tag{A.6}$$

References

[1] R. Bulirsch, Bemerkungen zur Romberg-Integration, *Numer. Math.* **6** (1964) 6–16.

[2] L. Fox, Romberg integration for a class of singular integrands, *The Computer Journal* **10** (1967) 87–93.

[3] J.N. Lyness, An error functional expansion for N-dimensional quadrature with an integrand function singular at a point, *Math. Comp.* **30** (1976) 1–23.

[4] J.N. Lyness and B.J.J. McHugh, On the remainder term in the N-dimensional Euler–Maclaurin Expansion, *Numer. Math.* **15** (1970) 333–344.

[5] J.N. Lyness and B.W. Ninham, Numerical quadrature and asymptotic expansions, *Math. Comp.* **21** (1967) 162–178.

[6] E.T. Whittaker and G.N. Watson, *A Course of Modern Analysis* (Cambridge University Press, New York, 1961).